

Harmonic oscillator well with a screened Coulombic core is quasi-exactly solvable

Miloslav Znojil

Ústav jaderné fyziky AV ČR, 250 68 Řež, Czech Republic

Abstract

In the quantization scheme which weakens the hermiticity of a Hamiltonian to its mere \mathcal{PT} invariance the superposition $V(x) = x^2 + Ze^2/x$ of the harmonic and Coulomb potentials is defined at the purely imaginary effective charges ($Ze^2 = if$) and regularized by a purely imaginary shift of x . This model is quasi-exactly solvable: We show that at each excited, $(N + 1)$ -st harmonic-oscillator energy $E = 2N + 3$ there exists not only the well known harmonic oscillator bound state (at the vanishing charge $f = 0$) but also a normalizable $(N + 1)$ -plet of the further elementary Sturmian eigenstates $\psi_{\{n\}}(x)$ at eigencharges $f = f_{\{n\}} > 0$, $n = 0, 1, \dots, N$. Beyond the smallest multiplicities N we recommend their perturbative construction.

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1 Introduction

Schrödinger equation for all the asymptotically harmonic oscillators in one dimension,

$$\left[-\frac{d^2}{dx^2} + x^2 + 2\alpha x - E + \mathcal{O}(1/x) \right] \psi(x) = 0, \quad (1)$$

need not necessarily be kept defined just on the real axis of coordinates. Indeed, its available physical asymptotic solutions

$$\psi(x) \sim \exp \left[-\frac{x^2}{2} - \alpha x + b \ln(x) + \mathcal{O}(1/x) \right], \quad b = (E + \alpha^2 - 1)/2 \quad (2)$$

are normalizable not only on the real intervals $x > x_a \gg 1$ and $x < -x_a$ but also in their complex vicinity defined by the respective formulae

$$|x| \in (x_a, \infty), \quad \arg x \in (-\pi/4, \pi/4) \quad \text{and} \quad \arg x \in (-5\pi/4, -3\pi/4). \quad (3)$$

One may connect these two complex wedges by a contour of integration which is arbitrarily deformed within the domain of analyticity of the potential in question. In particular, one may choose the purely harmonic $V(x) = x^2$ and move the real axis of coordinates x to a parallel line at a distance a . The new, shifted potential $V(x) = x^2 + 2aix - a^2$ loses its hermiticity and preserves only a certain symmetry with respect to a simultaneous change of the parity \mathcal{P} ($x \rightarrow -x$) and of the time ordering \mathcal{T} (which means the mere complex conjugation $i \rightarrow -i$ in time-independent cases), *without any change in the discrete spectrum itself*.

Similar paradoxes seem to have inspired a deeper analysis of the various \mathcal{PT} symmetric phenomenological models. Bessis and Zinn-Justin [1] related some of them to the so called Lee-Yang zeros in field theory [2] and Bender with coauthors paid attention to their possible role in the parity breaking [3], phase transitions [4] and quantum electrodynamics [5].

\mathcal{PT} symmetry does not prove less exciting on a purely methodical level. Its use may range from the fundamental problems of the ambiguities of quantization [6] and of the exact solvability and Darboux transformations [7] up to the questions of convergence of perturbation expansions [8]. In this context, there also appeared

an amazing discovery [9] of the so called quasi-exact (which means incomplete [10]) solvability of quartic oscillators.

In contrast to its unsolvable three-dimensional counterpart the latter quartic model did not contain the Coulombic component e^2/x [11]. In all the one-dimensional Hermitean models this term is routinely being omitted due to its strongly singular character in the origin. In the \mathcal{PT} -symmetric non-hermitean setting, nevertheless, a purely imaginary shift *could* regularize this singular term in principle. This was our main inspiration.

Even after the screening $x \rightarrow x - ic$ the persistent imaginary part of forces $V(x) \sim 1/(x - ic)$ would still violate unitarity and cause the predominance of unstable, resonant bound states. At this point we may recall the above-mentioned strategy which tries to compensate the instabilities by the constraint of \mathcal{PT} symmetry. This re-defines the electric charge. With real f in its effective \mathcal{PT} -symmetric value $Ze^2 \equiv if$ the nontrivial interaction model need not even contain the cubic and quartic terms. Its Schrödinger equation with the three real parameters a , f and c reads

$$\left[-\frac{d^2}{dx^2} + x^2 + 2iax + i\frac{f}{x - ic} \right] \psi(x) = E\psi(x), \quad \psi(\pm\infty) = 0, \quad (4)$$

and gives, presumably, a real and discrete spectrum of energies E .

In what follows, we shall re-examine eq. (4) from the point of view of its possible quasi-exact solvability. We shall be able to show that its elementary $(N + 1)$ -plets of Sturmian eigenstates exist at any $N = 0, 1, \dots$ (Section 2) and that their explicit construction (mediated by the vanishing of an $(N + 1) \times (N + 1)$ -dimensional secular determinant, see below) may be significantly facilitated via perturbative techniques (Section 3). A summary of our results will be outlined in Section 4.

2 Quasi-exact solutions

2.1 Taylor series and its termination

Equations (1) and (2) clarify the structure of all the normalizable solutions $\psi(x)$ of eq. (4) near $x = \pm\infty$. In the light of the identity $1/(x - ic) \equiv (x + ic)/(x^2 + c^2)$ our model remains smooth and regular at all the finite coordinates and everywhere off the complex pole of $V(x)$ at $x = ic$. In the vicinity of this complex point it is convenient to demand that our wave functions vanish, $\psi(x) \approx x - ic$. Having in mind the possible deformations of the contour of integration, such a requirement is immediately inspired by the universal and widely accepted regularization of Schrödinger equations near their strong singularities [12]. On this basis let us now try to solve our present Schrödinger bound state problem (4) by means of the following elementary harmonic-oscillator-like ansatz

$$\psi(x) = (c + ix) \exp\left[-\frac{x^2}{2} - iax\right] \varphi(x), \quad \varphi(x) = \sum_{n=0}^N h_n (ix)^n. \quad (5)$$

Such a terminating Taylor-series assumption fixes the energy (cf. eq. (2)),

$$E = 2N + a^2 + 3. \quad (6)$$

Its insertion in our differential Schrödinger bound state problem (4) leads to the equivalent $N + 1$ recurrence relations

$$A_n h_{n-1} + B_n h_n + C_n h_{n+1} + D_n h_{n+2} = 0, \quad n = 0, 1, \dots, N.$$

Keeping in mind that $h_{-1} = h_{N+1} = h_{N+2} = 0$ we easily derive the values of the coefficients,

$$\begin{aligned} D_n &= c(n+1)(n+2), & C_n &= (n+1)(n+2-2ac), \\ B_n &= -2a(n+1) - 2c(N+1-n) - f, & A_n &= -2(N+1-n). \end{aligned}$$

They may be arranged in a square matrix with four diagonals,

$$Q = \begin{pmatrix} B_0 & C_0 & D_0 & & & \\ A_1 & B_1 & C_1 & D_1 & & \\ & A_2 & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & D_{N-2} \\ & & & A_{N-1} & B_{N-1} & C_{N-1} \\ & & & & A_N & B_N \end{pmatrix}.$$

In notation with the row vectors $\vec{h} = (h_0, h_1, \dots, h_N)$ our recurrences may be then re-interpreted as a non-hermitean matrix problem

$$Q \vec{h}^T = 0.$$

Normalization $h_N = 1$ implies its immediate compact and unique solution

$$h_{N-k-1} = \frac{1}{2^{k+1} (k+1)!} \det \begin{pmatrix} B_{N-k} & C_{N-k} & D_{N-k} & & \\ A_{N-k+1} & \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots & D_{N-2} \\ & & A_{N-1} & B_{N-1} & C_{N-1} \\ & & & A_N & B_N \end{pmatrix} \quad (7)$$

for all the relevant indices $k = 0, 1, \dots, N-1$. At the remaining, “redundant” value of $k = N$ the left-hand-side symbol vanishes identically since, due to our assumptions, $h_{-1} \equiv 0$. With the linear charge-dependence in $B_n = B_n(f) = B_n(0) - f$ and in $Q = Q(f) = Q(0) - fI$ this is equivalent to the current secular equation

$$\det [Q(0) - fI] = 0. \quad (8)$$

As a polynomial constraint of the $(N+1)$ –st degree this determines an $(N+1)$ –plet of eigencouplings $f = f_{\{k\}}$. They are complex in general. In the spirit of our introductory remarks it only remains for us to demonstrate that all these roots are real (i.e., not breaking the overall \mathcal{PT} –symmetry of our model), in a certain sub-domain of parameters at least.

2.2 Full \mathcal{PT} symmetry in the large-screening domain

For convenience let us shift the variable $f = X + (N + 2)(c - a)$ and look at Table 1. It lists the explicit secular equations at the first few lowest integers N . From the Table we may infer that all the zeros $X_{\{n\}}$ and/or $f_{\{n\}}$ of eq. (8) are just functions of the single parameter $d = c + a$. This is not surprising. The change of the value of a is just a shift of the integration path within the domain of analyticity of our potential. We may demonstrate the explicit form of this type of invariance of our differential eq. (4) algebraically: The equation remains the same after we compensate the change of the coordinate $x \rightarrow x + i\delta$ by the simultaneous shift $a \rightarrow a + \delta$ and $c \rightarrow c - \delta$ of our pair of parameters. The values of f and d remain unchanged. In our subsequent considerations we shall put $a = 0$ without any loss of generality, therefore.

Assuming that the strong Coulomb singularity lies off the real line, $c \neq 0$, we may introduce $\lambda = 1/c$ and re-scale $Y = X/c$. Our secular equation (8) may be re-phrased as corresponding to the asymmetric linear algebraic problem

$$\begin{pmatrix} -Y - N & 2\lambda & 2 & & & \\ -2N\lambda & -Y - N + 2 & 6\lambda & 6 & & \\ & (2 - 2N)\lambda & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & N(N - 1) \\ & & & -4\lambda & -Y + N - 2 & N(N + 1)\lambda \\ & & & & -2\lambda & -Y + N \end{pmatrix} \begin{pmatrix} h_0 \\ h_1 \\ h_2 \\ \vdots \\ h_{N-1} \\ h_N \end{pmatrix} = 0. \quad (9)$$

In the large-displacement limit $\lambda \rightarrow 0$ we get an exactly solvable case which determines the real eigencharges $f_{\{n\}}$. This may be proved easily since in this limit our “Hamiltonian” $\lambda Q = H - Y I$ becomes an upper triangular matrix. This leads to the following closed formula

$$(Y_{\{0\}}, Y_{\{1\}}, \dots, Y_{\{N\}}) \rightarrow (Y_{\{0\}}^{[0]}, Y_{\{1\}}^{[0]}, \dots, Y_{\{N\}}^{[0]}) = (N, N - 2, \dots, -N + 2, -N)$$

which determines the real and approximately equidistant spectrum of eigencharges $f = f_{\{n\}}(c) = 2(n + 1)c + \mathcal{O}(1/c)$ with $n = 0, 1, \dots, N$.

3 Sturmian bound states at the general N

Once we fix the integer N and recall the nonlinear algebraic definition (8) of our $(N+1)$ eigencouplings $f = f_{\{n\}}$ we immediately imagine that the explicit construction of our Sturmians becomes more and more complicated for the larger dimensions N . Even if we extend, accordingly, the list of our secular polynomials in Table 1 we must necessarily resort to the purely numerical methods when trying to determine their exact roots f . The task is easy for the first few integers N only.

At the large N , our numerical algorithms may still start from the above equidistant asymptotic estimates and make use of the expected smooth change of the roots f with the decrease of the parameter $|d| < \infty$. Indeed, the boundary of the domain $d > d_{critical}(N)$ where all our roots f stay real is only slowly growing with N since $d_{critical}(1) = 2$, $d_{critical}(2) \approx 2.9865$, $d_{critical}(3) \approx 3.765$ etc.

All this indicates that in practice a perturbative evaluation of the eigencharges could prove almost as efficient as their direct numerical determination, especially beyond the smallest N .

3.1 Perturbation expansions with $\lambda < \lambda_{critical}$

The inspection of the (extended) Table 1 reveals that

$$Y(\lambda) = Y^{[0]} + \lambda^2 Y^{[2]} + \lambda^4 Y^{[4]} + \dots \quad (10)$$

This means that all the odd perturbation corrections vanish identically, $Y^{[2k+1]} = 0$. In the similar spirit we may also write

$$\vec{h} = \vec{h}(\lambda) = \vec{h}^{[0]} + \lambda \vec{h}^{[1]} + \lambda^2 \vec{h}^{[2]} + \dots \quad (11)$$

In order to appreciate the possible merits of such an approach let us return to our asymmetric eq. (9) and notice that at $\lambda = 0$ it decays into a direct sum of the two linear equations. Each of them couples only h_n 's with the same parity of the subscript n . This is a pleasant simplification. For example, the five-dimensional unperturbed eigenvalue problem at $N = 4$ decays into the separate two- and three-dimensional

sub-equations. We may omit the redundant superscripts ^[0] and display the latter subset for illustration,

$$\begin{pmatrix} -Y-4 & 2 & 0 \\ 0 & -Y & 12 \\ 0 & 0 & -Y+4 \end{pmatrix} \begin{pmatrix} h_0 \\ h_2 \\ h_4 \end{pmatrix} = 0. \quad (12)$$

Relaxing our above normalization convention and working in the integer arithmetics (i.e., in full precision, without any round-off errors) its first solution $\vec{h}_{\{a\}} = (1, 0, 0)$ is found for the eigencharge $Y = Y_{\{a\}} = -4$ while $\vec{h}_{\{b\}} = (1, 2, 0)$ is obtained at the vanishing $Y_{\{b\}} = 0$ and $\vec{h}_{\{c\}} = (3, 12, 4)$ results from $Y_{\{c\}} = +4$.

Returning to our matrix form $Q \vec{h}^T = 0$ of the differential Schrödinger eq. (4) with “Hamiltonian” $\lambda Q = H - Y I$ and decomposition $H = H^{[0]} + \lambda H^{[1]}$ at a general N we may now solve it by means of the textbook Rayleigh-Schrödinger perturbation theory [13]. In the present implementation of this recipe the k -th unknown perturbation corrections will be determined by the relation

$$\begin{aligned} & (H^{[0]} - Y^{[0]} I) (\vec{h}^{[k]})^T + (H^{[1]} - Y^{[1]} I) (\vec{h}^{[k-1]})^T - \\ & - Y^{[2]} (\vec{h}^{[k-2]})^T - \dots - Y^{[k]} (\vec{h}^{[0]})^T = 0. \end{aligned}$$

We have to solve it step-by-step, at all the subsequent perturbation orders $\mathcal{O}(\lambda^k)$ numbered by the integer $k = 1, 2, \dots$. For illustration let us pick up $N = 2$ and $Y^{[0]} = 2$. In the first-order approximation with $k = 1$ we normalize $h_N^{[1]} = 0$ and drop all the superscripts ^[1] from $Y^{[1]}$ and $\vec{h}^{[1]}$. The perturbed equation (9) then acquires its $\mathcal{O}(\lambda)$ first-order form

$$\begin{pmatrix} -4 & 0 & +2 \\ 0 & -2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} h_0 \\ h_1 \\ 0 \end{pmatrix} + \begin{pmatrix} -Y & 2 & 0 \\ -4 & -Y & 6 \\ 0 & -2 & -Y \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 2 \end{pmatrix} = 0.$$

This implies that $Y = Y^{[1]} = 0$ (as expected) and $\vec{h} = \vec{h}^{[1]} = (0, 4, 0)$. By the way, the latter result nicely illustrates a general feature: We might replace eq. (11) by a component-by-component expansion in the powers of squares λ^2 in a way paralleling the expansion of charges Y above. This reflects a symmetry of our model with respect to the change of sign of the parameter of screening d .

3.2 The role of asymmetry

We have established that our recurrences (9) provide a new, not entirely standard framework for application of perturbation theory. The manifestly non-hermitean two-diagonal structure of the underlying exactly solvable unperturbed Hamiltonians $H^{[0]}$ requires a modification of the formalism itself. The necessity of re-considering the standard concepts (say, of the model-space projector) seems to deserve a separate comment. The point is that due to the manifest difference between our original and transposed pseudo-Hamiltonians we must consider not only the “direct” zero-order eigenvalue problem $[Q(0) - f I] (\vec{h}^{[0]})^T = 0$ (or rather equation

$$(H^{[0]} - Y_{\{\alpha\}} I) (\vec{h}_{\{\alpha\}}^{[0]})^T = 0$$

at a fixed subscript $\alpha = 0, 1, \dots, N$) but also its transposed, non-equivalent pendant

$$\left[(H^{[0]})^T - Y_{\{\alpha\}} I \right] (\vec{g}_{\{\alpha\}}^{[0]})^T = 0.$$

It is worth noticing that in a way paralleling eq. (7) above, all the left eigenvectors $\vec{g} = \vec{g}(\lambda)$ may be defined by closed formulae,

$$g_{k+1} = \frac{(N-k-1)!}{2^{k+1} (k+1)!} \det \begin{pmatrix} B_0 & C_0 & D_0 & & \\ A_1 & \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots & D_{k-2} \\ & & A_{k-1} & B_{k-1} & C_{k-1} \\ & & & A_k & B_k \end{pmatrix}.$$

Their knowledge would simplify the large-order algorithm. Still, due to the unphysical, auxiliary character of all the left eigenvectors, it is shorter to generate and use them just in the zero order. Dropping their superscript $^{[0]}$ as redundant, we may return to our illustration (12) and complement it by the left eigenvectors $\vec{g}_{\{a\}} = (4, -2, 3)$, $\vec{g}_{\{b\}} = (0, 1, -3)$ and $\vec{g}_{\{c\}} = (0, 0, 1)$. Incidentally, the overlaps $G = (g, h)$ form a diagonal matrix, $G_{11} = G_{33} = 4$, $G_{22} = 2$. This trivializes $F = G^{-1}$ needed in the model-space projectors $P_{\{\alpha\}} = \vec{h}_{\{\alpha\}}^T F_{\alpha, \alpha} \vec{g}_{\{\alpha\}}$. They are, counter-intuitively, non-diagonal but compatible with the usual completeness relation $I = \sum_{\alpha, \beta} \vec{h}_{\{\alpha\}}^T F_{\alpha, \beta} \vec{g}_{\{\beta\}}$.

4 Concluding remarks

4.1 Sturmians and the algebra $sl(2)$.

Our wave function (5) becomes purely real after the change of variables $x = -iy$ which rotates the axes by $\pi/2$. Of course, the exponential growth of our asymptotics (2) in the new artificial variable y has no meaning at all and only the original coordinate x remains physical. Still, the use of y simplifies our ansatz (5). With $a = 0$ it leads to a new differential Schrödinger equation $\hat{H}\hat{\varphi}(y) = f\hat{\varphi}(y)$ for real polynomials $\hat{\varphi}(y) = \varphi(-iy)$ themselves. In this notation our third Hamiltonian-like operator \hat{H} is the quadratic function of generators of the complex $sl(2)$ Lie algebra,

$$\hat{H} = \mathcal{J}^0 \mathcal{J}^- + 2\mathcal{J}^+ - 2c\mathcal{J}^0 + (N+2)\mathcal{J}^- - 2(N+c)$$

with

$$\begin{aligned} [\mathcal{J}^- \mathcal{J}^0] &= \mathcal{J}^- = \frac{d}{dy}, \\ [\mathcal{J}^- \mathcal{J}^+] &= 2\mathcal{J}^0 = 2(y+c)\frac{d}{dy} - 2N, \\ [\mathcal{J}^0 \mathcal{J}^+] &= \mathcal{J}^+ = (y+c)^2\frac{d}{dy} - 2(y+c)N. \end{aligned}$$

This fits the general scheme [14], parallels closely the similar quartic-oscillator result of ref. [9] (with the same algebra but different \hat{H}) and re-confirms our above conclusion that in spite of its non-hermiticity, our \mathcal{PT} -symmetric Schrödinger eq. (4) is quasi-exactly solvable.

In this context, we would like to emphasize that there exists a nice parallel between the Hermitean and \mathcal{PT} -symmetric quasi-exactly solvable models. Picking up the characteristic examples and adding our present results, we may now summarize and list the following four different possibilities and types of the quasi-exact constructions.

- The characteristic polynomial example $V(x) = \alpha x^2 + \beta x^4 + x^6$ with a constrained variability, say, of the coupling α leads to the existence of some N elementary bound states at a finite multiplet of the binding energies in the hermitean case [15].

- With a constrained variability of the energy E the non-polynomial hermitean potentials exemplified by $V(r) = x^2 + \alpha/(1 + \beta x^2)$ lead to the elementary Sturmian solutions at a finite N -plet of couplings α [16].
- In the \mathcal{PT} -symmetric case, the complex quartic polynomial potential of ref. [9], $V(x) = \alpha x + \beta x^2 + \gamma x^3 - x^4$ with a constrained variability of α , exhibits the quasi-exact solvability of the sextic-oscillator type.
- $V(x) = x^2 + i\alpha x + i\beta(x + i\gamma)/(x^2 + \gamma^2)$ of the present model (4) is the “missing” \mathcal{PT} -symmetric partner to the quasi-exact solvability of the non-polynomial Sturmian type.

4.2 Complex charges

We have seen that the one-dimensional Schrödinger equation becomes quasi-exactly solvable for Coulomb plus harmonic superpositions of potentials provided only that we regularize these forces in the \mathcal{PT} -symmetric manner. Multiplets of the Sturmian eigenstates acquire then an elementary polynomial form at certain purely imaginary couplings $Ze^2 = i f_{\{n\}}$ at $n = 0, 1, \dots, N$ and any $N = 0, 1, \dots$

In a tentative physical support of these *complex* electric charges we might recall a few of their \mathcal{PT} symmetric predecessors. A close connection exists with the Bessis’ cubic force possessing a purely imaginary coupling $g = i f$. Its rigorous mathematical analysis has already been delivered, many years ago, by Calicetti et al [17]. One may also mention an even closer parallel with the Bender’s and Milton’s electrodynamics which replaces, for several independent reasons [5], the charge e itself (i.e., not its present square e^2) by a purely imaginary quantity.

In a broader methodical context, our new phenomenological model (4) extends the family of potentials which are comparatively easily described in the language of analytic continuations [18]. Its distinctive feature, in this setting, is the presence of a complex pole. Its most important formal merit is its quasi-exact solvability shared with the quartic model of ref. [9]. In the latter comparison, one could emphasize the

“more natural” asymptotic behaviour of our present wave functions: The real axis of coordinates still lies within the wedges (3) of the admissible analytic continuations.

In the context of perturbative considerations it is amusing to notice that a “nice” (which means real, discrete and bounded) character of spectrum of our present \mathcal{PT} symmetric model may be viewed as a result of perturbation of *any* one of its *two* exactly solvable halves.

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Table 1. The first six secular equations (8) for eigencharges $f + (N+2)(a-c) \equiv X$, with a variable parameter $c + a \equiv d$ and abbreviation $d^2 - N - 3 \equiv h$.

N	$\det Q(f) = 0$
0	$-X = 0$
1	$X^2 - h = 0$
2	$-X^3 + 4hX + 8d = 0$
3	$X^4 - 10hX^2 - 48dX + 9h^2 - 36 = 0$
4	$-X^5 + 20hX^3 + 168dX^2 - 32(2h^2 - 9)X - 384hd = 0$
5	$X^6 - 35hX^4 - 448dX^3 + (259h^2 - 1296)X^2 +$ $+3520hdX - 225h^3 + 10000h + 51200 = 0$

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